Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

Bis(8-methylquinolinium) tetrabromidoferrate(III) bromide

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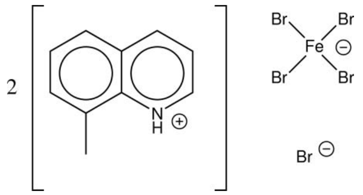
Received 15 May 2007; accepted 16 May 2007

Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.005 Å; R factor = 0.023; wR factor = 0.057; data-to-parameter ratio = 17.0.

The asymmetric unit of the title compound, $(C_{10}H_{10}N)_2[FeBr_4]Br$, contains two protonated 8-methylquinolinium cations, one bromide anion and one tetrabromidoferrate anion. The mean Fe—Br distance is 2.3338 (6) Å. The 8-methylquinolinium cations are planar and are inclined at a dihedral angle of 5.25 (9)° with respect to each other. The two 8-methylquinolinium cations and bromide anion are connected *via* N—H···Br hydrogen bonds. Furthermore, there are short C—H···Br contacts and $\pi\cdots\pi$ stacking interactions between cations. The N—H···Br hydrogen bonds link the molecules into chains along the [210] direction.

Related literature

For details of other tetrahalidoferrates with quinoline and its derivatives, see: Bottomley *et al.* (1984), Warnke *et al.* (2006), Wyrzykowski, Sikorski, Konitz *et al.* (2006), Wyrzykowski, Sikorski, Lis *et al.* (2006), Wyrzykowski, Warnke *et al.* (2006); and for similar tetrahalidoferrates with aromatic amines acting as balancing cations, see: Abboud *et al.* (2005), Barbaro *et al.* (1992), Chan & Baird (2004), Couce *et al.* (1995), Daran *et al.* (1979), James *et al.* (2001), James *et al.* (1982), Khan *et al.* (1987), Lowe *et al.* (1990), Lowe *et al.* (1994), Hackert & Jacobson (1971), Podesta & Orpen (2005), Shaviv *et al.* (1992), Veidis *et al.* (1979), Veidis *et al.* (1981), Zora *et al.* (1990), Zordan *et al.* (2005). For general synthetic procedures, see: Warnke *et al.* (2003). See also: Desiraju & Steiner (1999).



Experimental

Crystal data

$(C_{10}H_{10}N)_2[FeBr_4]Br$
M_r = 743.78
Triclinic, $P\overline{1}$
a = 7.9533 (5) Å
b = 10.3853 (4) Å
c = 15.2432 (8) Å
α = 84.781 (4)°
β = 79.645 (5)°
γ = 85.556 (4)°
V = 1231.00 (11) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 8.74 mm^{-1}
T = 291.2 (3) K
0.38 × 0.11 × 0.03 mm

Data collection

Kuma KM4 CCD diffractometer
Absorption correction: numerical *X-RED* (Stoe & Cie, 1999)
T_{min} = 0.321, T_{max} = 0.780
12314 measured reflections
4345 independent reflections
3120 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.057
S = 0.98
4345 reflections
255 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.57 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1N···Br99^{i}	0.96	2.39	3.229 (2)	146
N11—H11N···Br99	0.98	2.25	3.168 (3)	155
C10—H10A···Br99^{ii}	0.96	2.89	3.819 (4)	163

Symmetry codes: (i) $x, y+1, z$; (ii) $-x+1, -y+1, -z+1$.

Table 2
Geometry of stacking interactions (Å, °).

$Cg(Z)$ is the centroid of the six-membered ring containing atom Z. $Cg\cdots Cg$ is the distance between ring centroids, α is the dihedral angle between planes I and J, β is the angle between the $Cg(I)\rightarrow Cg(J)$ vector and the normal to plane I, γ is the angle between the $Cg(I)\rightarrow Cg(J)$ vector and the normal to plane J, $Cg(I)_p$ is the perpendicular distance of $Cg(I)$ from ring J and $Cg(J)_p$ is the perpendicular distance of $Cg(J)$ from ring I.

$Cg(I)\cdots Cg(J)$	$Cg\cdots Cg$	α	β	γ	$Cg(I)_p$	$Cg(J)_p$
Cg(N1)···Cg(C19)	3.8970	5.16	25.25	30.36	3.363	3.525
Cg(C9)···Cg(N11)	3.8130	5.14	26.19	21.42	3.550	3.421
Cg(C9)···Cg(C19)	3.7089	4.14	17.96	17.24	3.542	3.528

Data collection: *CrysAlis CCD* (UNIL IC & Kuma 2000); cell refinement: *CrysAlis RED* (UNIL IC & Kuma 2000); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL/PC* (Sheldrick, 1990*b*), *ORTEP-3* (Farrugia 1997); software used to prepare material for publication: *SHELXL97* (Sheldrick, 1997) and *PLATON* (Spek, 2003).

This work was supported by the Polish State Committee for Scientific Research (grant No. DS/8230-4-0088-7). The crystallographic part was financed by funds allocated by the Ministry of Science and Higher Education to the Institute of General and Ecological Chemistry, Technical University of Łódź, Poland.

doi:10.1107/S160053680702418X

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2370).

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supplementary materials

Acta Cryst. (2007). E**63**, m1727-m1728   [**doi:10.1107/S160053680702418X**]

Bis(8-methylquinolinium) tetrabromidoferrate(III) bromide

R. Kruszynski, **D. Wyrzykowski** and **L. Chmurzynski**

Comment

The composition of quinolinium and methylquinolinium tetrahalogenoferrates(III) has been found to be distinctly dependent on location of the methyl substituent in the quinoline ring and the kind of halide ligands in the coordination sphere of Fe(III) (Warnke *et al.*, 2003). When a quinolinum cation is a counter-ion, both the $[FeBr_4]^-$ and $[FeCl_4]^-$ anions form binary (1:1) salts (Wyrzykowski, Sikorski, Konitz *et al.*, 2006). With a 2-methyl substituted quinolinium cation, resulting salts have a composition of (2MeQH)2[FeX4]*X* (where 2MeQH is 2-methylquinolinum cation, and *X* = Br or Cl) (Warnke *et al.*, 2006; Wyrzykowski, Sikorski, Lis *et al.*, 2006). Introduction of the 2-methylquinoline substituted at position 4 by —NH_2 leads again to formation of 1:1 salt (Wyrzykowski, Warnke *et al.*, 2006). Thus determining the composition of $FeBr_4$ complex containing quinoline methylated at another position was interesting, and in future can lead to general conclusions about influence of quinoline substituents on complex composition.

All 8-methylquinolinium cations intramolecular distances and angles in (I) (Fig. 1) can be considered normal. All atoms lie in general positions. The asymmetric unit contains two protonated 8-methylquinolinium cations, one bromide anion and one tetrabromoferrate anion. The mean Fe—Br distance is 2.3338 (6) Å. Two Br—Fe—Br angles are smaller than tetrahedral, two are almost tetrahedral, and two are greater than tetrahedral. The 8-methylquinolinium cations can be considered planar and are inclined at 5.25 (9)°. From weighted least-squares planes calculated through all non-hydrogen atoms of the cations the most deviating atoms are C7 [0.025 (3) Å] in one molecule and C14 [0.026 (3) Å] in the second molecule. The two 8-methylquinolinium cations and bromide anion are connected *via* N—H···Br hydrogen bonds (Table 1, Fig. 2). In the structure can be found one more intermolecular C—H···Br short contact (Table 2), which, according to Desiraju & Steiner (1999), can be considered as a weak hydrogen bond. The cations are associated *via* π···π stacking interactions (Table 2) to dimers, and dimers are separated by anions one form each other. Thus, in considered structure, tetrabromoferrate anions play role of stacking breaker. The N—H···Br hydrogen bonds link the molecules to a chain running along [2 1 0] (Fig. 2).

Experimental

To a solution of $FeBr_3$ (*ca* 0.025 mol) in ethanol (96%) (50 ml), a stoichiometric quantity of a 40% HBr solution and 8-methylquinoline (*ca* 0.025 mol) were added in turn. The compound crystallized directly from the reaction mixture at ambient temperature. After *ca* 3 months dark-red crystals appeared. The compound was dried over P_4O_{10} in a vacuum desiccator. Elemental analysis (calculated/found %): C 32.38/32.28, H 2.69/2.66, N 3.77/3.80, Br 53.74/53.54, Fe 7.51/7.28.

Refinement

The carbon-bonded hydrogen atoms were placed in calculated positions and were refined as riding on adjacent carbon atom with fixed U values [$U_{iso}(H) = 1.2U_{eq}(C)$ or $U_{iso}(H) = 1.5U_{eq}(C\text{-methyl})$]. The methyl groups were allowed to rotate about their local threefold axis (AFIX 137). The nitrogen-bonded hydrogen atoms were founded from difference Fourier synthesis after eight cycles of anisotropic refinement and were refined as riding on adjacent nitrogen atom with fixed U values ($U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(N).

Figures

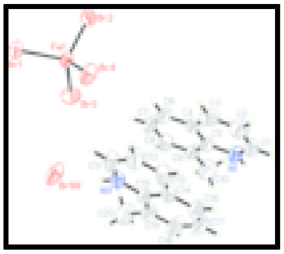

Fig. 1. Molecular structure of the title compound (I). Displacement ellipsoids are drawn at the 50% probability level.

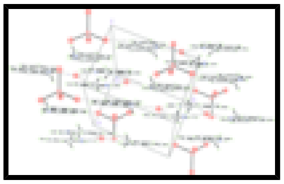

Fig. 2. A part of the molecular packing of the title compound showing short intermolecular interactions (hydrogen bonds are indicated by dashed lines).

Bis(8-methylquinolinium) tetrabromidoferrate(III) bromide

Crystal data

$(C_{10}H_{10}N)_2[FeBr_4]Br$
$M_r = 743.78$
Triclinic, $P\bar{1}$
Hall symbol: -P 1
$a = 7.9533$ (5) Å
$b = 10.3853$ (4) Å
$c = 15.2432$ (8) Å
$\alpha = 84.781$ (4)°
$\beta = 79.645$ (5)°
$\gamma = 85.556$ (4)°
$V = 1231.00$ (11) Å^3

$Z = 2$
$F_{000} = 710$
$D_x = 2.007$ Mg m^{-3}
$D_m = 2.01$ Mg m^{-3}
D_m measured by Berman density torsion balance
Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 7884 reflections
$\theta = 5$–20°
$\mu = 8.74$ mm^{-1}
$T = 291.2$ (3) K
Plate, orange
0.38 × 0.11 × 0.03 mm

Data collection

Kuma KM4-CCD diffractometer
Radiation source: fine-focus sealed tube
Monochromator: graphite
Detector resolution: 1048576 pixels mm^{-1}
$T = 291.2(3)$ K
ω scans

4345 independent reflections
3120 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.020$
$\theta_{\rm max} = 25.1$°
$\theta_{\rm min} = 2.0$°
$h = -8\rightarrow9$

Absorption correction: numerical X-RED. STOE & Cie (1999)

$T_{\min} = 0.321$, $T_{\max} = 0.780$

12314 measured reflections

$k = -12 \rightarrow 12$

$l = -16 \rightarrow 18$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.023$

$wR(F^2) = 0.057$

$S = 0.98$

4345 reflections

255 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0304P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 0.43$ e Å^{-3}

$\Delta\rho_{\min} = -0.57$ e Å^{-3}

Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against all reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on all data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Fe1	0.84814 (6)	0.24354 (4)	0.12389 (3)	0.04493 (13)
Br1	0.82953 (4)	0.02568 (3)	0.10380 (2)	0.05566 (11)
Br2	1.10108 (4)	0.31300 (3)	0.03423 (2)	0.05990 (11)
Br4	0.61015 (5)	0.36204 (4)	0.08073 (3)	0.06862 (13)
Br5	0.86151 (6)	0.26018 (5)	0.27339 (3)	0.08107 (14)
N1	0.4142 (3)	1.0191 (2)	0.24958 (17)	0.0491 (7)
H1N	0.4300	1.0708	0.2958	0.059*
C1	0.3428 (4)	1.0733 (3)	0.1817 (2)	0.0580 (9)
H1	0.2962	1.1582	0.1832	0.070*
C2	0.3373 (4)	1.0048 (4)	0.1094 (2)	0.0654 (10)
H2	0.2877	1.0430	0.0617	0.078*
C3	0.4047 (4)	0.8812 (4)	0.1083 (2)	0.0610 (10)
H3	0.4010	0.8348	0.0594	0.073*
C4	0.4800 (4)	0.8217 (3)	0.1789 (2)	0.0498 (8)

C5	0.4844 (4)	0.8946 (3)	0.2527 (2)	0.0461 (8)
C6	0.5485 (4)	0.6941 (4)	0.1818 (3)	0.0634 (10)
H6	0.5488	0.6445	0.1340	0.076*
C7	0.6143 (5)	0.6420 (4)	0.2538 (3)	0.0780 (13)
H7	0.6563	0.5559	0.2557	0.094*
C8	0.6205 (4)	0.7161 (4)	0.3261 (3)	0.0680 (11)
H8	0.6685	0.6782	0.3743	0.082*
C9	0.5574 (4)	0.8425 (3)	0.3269 (2)	0.0543 (9)
C10	0.5637 (5)	0.9234 (4)	0.4024 (2)	0.0799 (12)
H10A	0.6154	0.8724	0.4474	0.120*
H10B	0.4495	0.9531	0.4277	0.120*
H10C	0.6301	0.9966	0.3804	0.120*
N11	0.1901 (3)	0.5284 (2)	0.31091 (18)	0.0494 (7)
H11N	0.2398	0.4574	0.3473	0.059*
C11	0.1751 (4)	0.5010 (3)	0.2300 (2)	0.0581 (9)
H11	0.2104	0.4188	0.2116	0.070*
C12	0.1075 (5)	0.5929 (3)	0.1723 (3)	0.0648 (10)
H12	0.0967	0.5732	0.1153	0.078*
C13	0.0573 (4)	0.7127 (3)	0.2003 (2)	0.0603 (9)
H13	0.0107	0.7750	0.1622	0.072*
C14	0.0747 (4)	0.7440 (3)	0.2859 (2)	0.0502 (8)
C15	0.1451 (4)	0.6474 (3)	0.3433 (2)	0.0456 (8)
C16	0.0312 (5)	0.8670 (4)	0.3157 (3)	0.0669 (10)
H16	−0.0146	0.9320	0.2792	0.080*
C17	0.0557 (5)	0.8919 (4)	0.3977 (3)	0.0823 (12)
H17	0.0274	0.9744	0.4172	0.099*
C18	0.1232 (5)	0.7949 (4)	0.4539 (3)	0.0826 (13)
H18	0.1367	0.8146	0.5105	0.099*
C19	0.1701 (4)	0.6718 (3)	0.4288 (2)	0.0624 (10)
C20	0.2449 (5)	0.5689 (4)	0.4901 (2)	0.0845 (13)
H20A	0.2644	0.6069	0.5422	0.127*
H20B	0.3514	0.5326	0.4591	0.127*
H20C	0.1663	0.5018	0.5078	0.127*
Br99	0.31991 (6)	0.24911 (4)	0.38250 (3)	0.08361 (16)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Fe1	0.0569 (3)	0.0382 (3)	0.0423 (3)	0.0022 (2)	−0.0162 (2)	−0.0065 (2)
Br1	0.0671 (2)	0.03822 (19)	0.0643 (2)	−0.00061 (16)	−0.01844 (18)	−0.00616 (16)
Br2	0.0676 (2)	0.0539 (2)	0.0579 (2)	−0.00829 (17)	−0.01148 (18)	0.00184 (17)
Br4	0.0731 (3)	0.0532 (2)	0.0841 (3)	0.01958 (18)	−0.0308 (2)	−0.0154 (2)
Br5	0.1119 (3)	0.0926 (3)	0.0433 (2)	−0.0105 (3)	−0.0195 (2)	−0.0148 (2)
N1	0.0650 (17)	0.0445 (16)	0.0415 (16)	0.0087 (13)	−0.0197 (14)	−0.0121 (13)
C1	0.068 (2)	0.049 (2)	0.058 (2)	0.0062 (17)	−0.0183 (19)	−0.0016 (18)
C2	0.075 (3)	0.076 (3)	0.050 (2)	−0.005 (2)	−0.0211 (19)	−0.009 (2)
C3	0.068 (2)	0.076 (3)	0.044 (2)	−0.012 (2)	−0.0102 (18)	−0.0240 (19)
C4	0.049 (2)	0.050 (2)	0.050 (2)	−0.0086 (16)	−0.0003 (16)	−0.0152 (17)

C5	0.052 (2)	0.0398 (19)	0.046 (2)	0.0022 (15)	−0.0082 (16)	−0.0071 (15)
C6	0.059 (2)	0.048 (2)	0.081 (3)	−0.0017 (18)	0.002 (2)	−0.022 (2)
C7	0.070 (3)	0.036 (2)	0.120 (4)	0.0106 (18)	0.004 (3)	−0.014 (2)
C8	0.066 (2)	0.056 (2)	0.076 (3)	0.0125 (19)	−0.009 (2)	0.005 (2)
C9	0.060 (2)	0.048 (2)	0.053 (2)	0.0083 (17)	−0.0103 (18)	−0.0062 (17)
C10	0.103 (3)	0.088 (3)	0.055 (3)	0.018 (2)	−0.038 (2)	−0.009 (2)
N11	0.0596 (17)	0.0384 (15)	0.0500 (18)	0.0000 (13)	−0.0139 (14)	0.0033 (13)
C11	0.081 (3)	0.042 (2)	0.058 (2)	−0.0044 (17)	−0.026 (2)	−0.0095 (17)
C12	0.095 (3)	0.052 (2)	0.056 (2)	−0.009 (2)	−0.036 (2)	0.0004 (18)
C13	0.071 (2)	0.048 (2)	0.065 (3)	0.0004 (18)	−0.029 (2)	0.0077 (18)
C14	0.052 (2)	0.045 (2)	0.053 (2)	0.0009 (16)	−0.0101 (17)	−0.0005 (16)
C15	0.0498 (19)	0.0401 (19)	0.045 (2)	0.0051 (15)	−0.0052 (15)	−0.0038 (15)
C16	0.079 (3)	0.053 (2)	0.062 (3)	0.0169 (19)	−0.004 (2)	−0.0021 (19)
C17	0.110 (3)	0.058 (3)	0.072 (3)	0.022 (2)	0.000 (2)	−0.020 (2)
C18	0.120 (3)	0.074 (3)	0.049 (2)	0.023 (3)	−0.007 (2)	−0.021 (2)
C19	0.078 (3)	0.056 (2)	0.049 (2)	0.0091 (19)	−0.0057 (19)	−0.0054 (18)
C20	0.128 (4)	0.077 (3)	0.052 (2)	0.016 (3)	−0.032 (2)	−0.006 (2)
Br99	0.1428 (4)	0.0520 (2)	0.0567 (3)	0.0362 (2)	−0.0337 (3)	−0.01146 (19)

Geometric parameters (Å, °)

Fe1—Br5	2.3230 (6)	C10—H10B	0.9600
Fe1—Br1	2.3300 (5)	C10—H10C	0.9600
Fe1—Br4	2.3387 (5)	N11—C11	1.318 (4)
Fe1—Br2	2.3436 (6)	N11—C15	1.370 (4)
N1—C1	1.329 (4)	N11—H11N	0.9828
N1—C5	1.368 (4)	C11—C12	1.383 (4)
N1—H1N	0.9551	C11—H11	0.9300
C1—C2	1.374 (4)	C12—C13	1.359 (5)
C1—H1	0.9300	C12—H12	0.9300
C2—C3	1.353 (5)	C13—C14	1.405 (5)
C2—H2	0.9300	C13—H13	0.9300
C3—C4	1.398 (5)	C14—C16	1.393 (4)
C3—H3	0.9300	C14—C15	1.420 (4)
C4—C6	1.393 (5)	C15—C19	1.401 (4)
C4—C5	1.418 (4)	C16—C17	1.350 (5)
C5—C9	1.410 (4)	C16—H16	0.9300
C6—C7	1.351 (5)	C17—C18	1.401 (5)
C6—H6	0.9300	C17—H17	0.9300
C7—C8	1.409 (5)	C18—C19	1.373 (5)
C7—H7	0.9300	C18—H18	0.9300
C8—C9	1.369 (5)	C19—C20	1.512 (5)
C8—H8	0.9300	C20—H20A	0.9600
C9—C10	1.494 (5)	C20—H20B	0.9600
C10—H10A	0.9600	C20—H20C	0.9600
Br5—Fe1—Br1	107.92 (2)	C9—C10—H10C	109.5
Br5—Fe1—Br4	112.12 (2)	H10A—C10—H10C	109.5
Br1—Fe1—Br4	108.87 (2)	H10B—C10—H10C	109.5
Br5—Fe1—Br2	109.50 (2)	C11—N11—C15	123.8 (3)

Br1—Fe1—Br2	107.98 (2)	C11—N11—H11N	115.3
Br4—Fe1—Br2	110.33 (2)	C15—N11—H11N	120.9
C1—N1—C5	123.2 (3)	N11—C11—C12	120.8 (3)
C1—N1—H1N	119.6	N11—C11—H11	119.6
C5—N1—H1N	116.8	C12—C11—H11	119.6
N1—C1—C2	120.5 (3)	C13—C12—C11	118.7 (3)
N1—C1—H1	119.8	C13—C12—H12	120.6
C2—C1—H1	119.8	C11—C12—H12	120.6
C3—C2—C1	119.2 (3)	C12—C13—C14	121.1 (3)
C3—C2—H2	120.4	C12—C13—H13	119.5
C1—C2—H2	120.4	C14—C13—H13	119.5
C2—C3—C4	121.5 (3)	C16—C14—C13	122.8 (3)
C2—C3—H3	119.2	C16—C14—C15	118.5 (3)
C4—C3—H3	119.2	C13—C14—C15	118.7 (3)
C6—C4—C3	123.8 (3)	N11—C15—C19	121.0 (3)
C6—C4—C5	118.0 (3)	N11—C15—C14	116.8 (3)
C3—C4—C5	118.2 (3)	C19—C15—C14	122.1 (3)
N1—C5—C9	120.5 (3)	C17—C16—C14	119.9 (4)
N1—C5—C4	117.4 (3)	C17—C16—H16	120.0
C9—C5—C4	122.1 (3)	C14—C16—H16	120.0
C7—C6—C4	120.3 (3)	C16—C17—C18	120.8 (4)
C7—C6—H6	119.8	C16—C17—H17	119.6
C4—C6—H6	119.8	C18—C17—H17	119.6
C6—C7—C8	121.1 (3)	C19—C18—C17	122.5 (4)
C6—C7—H7	119.4	C19—C18—H18	118.7
C8—C7—H7	119.4	C17—C18—H18	118.7
C9—C8—C7	121.4 (4)	C18—C19—C15	116.2 (3)
C9—C8—H8	119.3	C18—C19—C20	121.7 (4)
C7—C8—H8	119.3	C15—C19—C20	122.1 (3)
C8—C9—C5	116.9 (3)	C19—C20—H20A	109.5
C8—C9—C10	122.5 (3)	C19—C20—H20B	109.5
C5—C9—C10	120.6 (3)	H20A—C20—H20B	109.5
C9—C10—H10A	109.5	C19—C20—H20C	109.5
C9—C10—H10B	109.5	H20A—C20—H20C	109.5
H10A—C10—H10B	109.5	H20B—C20—H20C	109.5

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1N···Br99^{i}	0.96	2.39	3.229 (2)	146
N11—H11N···Br99	0.98	2.25	3.168 (3)	155
C10—H10A···Br99^{ii}	0.96	2.89	3.819 (4)	163

Symmetry codes: (i) *x*, *y*+1, *z*; (ii) −*x*+1, −*y*+1, −*z*+1.

Stacking interactions geometry, distances in Å, angles in °. Cg(Z) means six-membered ring containing Z atom.

Cg(I)···*Cg*(J)	*Cg*···*Cg*	α	β	γ	*Cg*(I)$_p$	*Cg*(J)$_p$
Cg(N1)···*Cg*(C19)	3.8970	5.16	25.25	30.36	3.363	3.525
Cg(C9)···*Cg*(N11)	3.8130	5.14	26.19	21.42	3.550	3.421

Cg(C9)···*Cg*(C19)	3.7089	4.14	17.96	17.24	3.542	3.528

Cg···*Cg* - distance between ring centroids, α - dihedral Angle between Planes I and J, β - angle between *Cg*(I)-->*Cg*(J) vector and normal to plane I, γ - angle between *Cg*(I)-->*Cg*(J) vector and normal to plane J, *Cg*(I)$_{\mathrm{p}}$ perpendicular distance of *Cg*(I) on ring J, *Cg*(J)$_{\mathrm{p}}$ perpendicular distance of *Cg*(J) on ring I.

Fig. 1

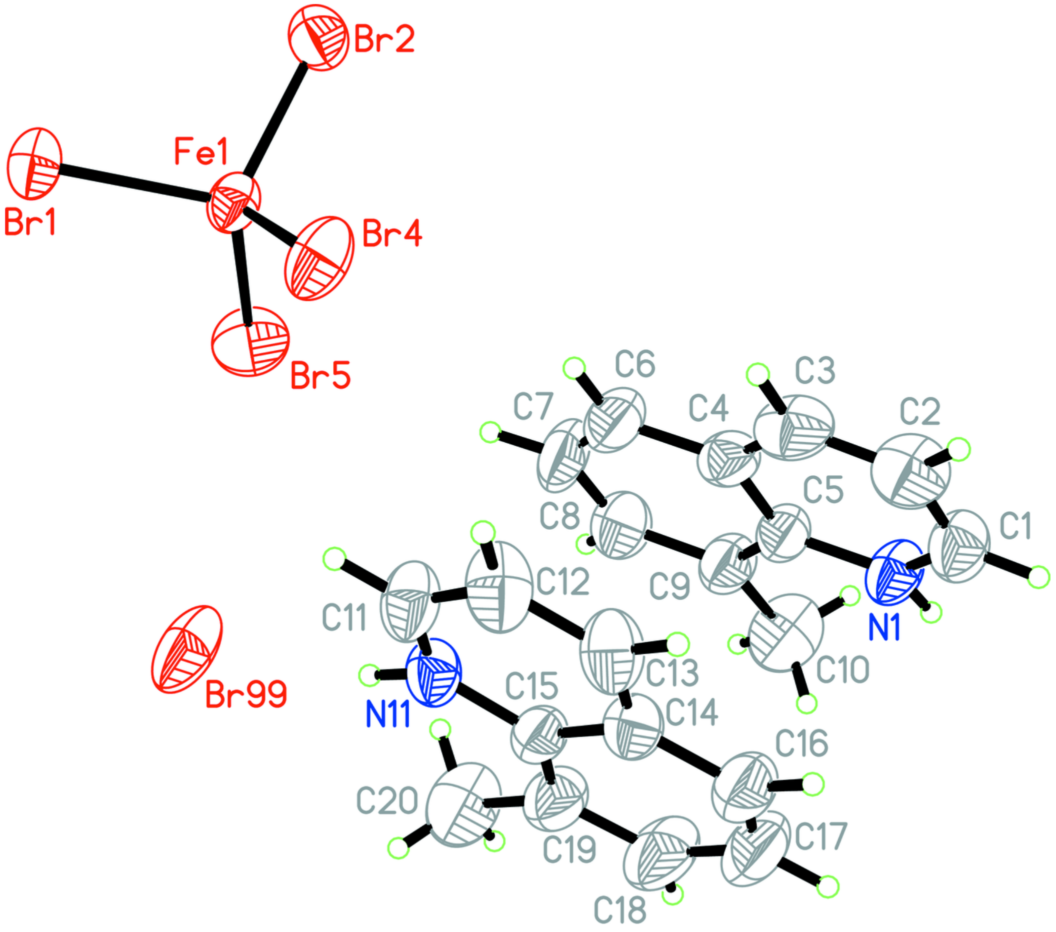
Br2
Fe1
Br1
Br4
Br5
C6
C3
C7
C4
C2
C5
C8
C1
C12
C9
C11
N1
C13
C10
Br99
C15
C14
N11
C16
C20
C17
C19
C18

Fig. 2